(3) Matrix Representation.

Operator X, ket $|a\rangle$, bra $\langle a|$,

.... How can we write them in "numbers"?

(like a wave function, for example.)

$\Rightarrow$
- Operator $X \doteq$ Matrix. $\begin{pmatrix} \diagdown \end{pmatrix}$
- ket $|a\rangle \doteq$ Column vector. (matrix) $\begin{pmatrix} | \end{pmatrix}$
- bra $\langle a| \doteq$ row vector (matrix). $\begin{pmatrix} — \end{pmatrix}$

· Operator $\quad X = I \cdot X \cdot I = \sum_i |i\rangle\langle i| \, X \, \sum_j |j\rangle\langle j|$

$$= \sum_{i,j} |i\rangle \underbrace{\langle i| X |j\rangle}_{\text{a matrix}} \langle j|$$

$$X \doteq \begin{array}{c|c} & \text{col. } j \rightarrow \\ \hline \text{row } i \downarrow & \begin{pmatrix} \langle 1|X|1\rangle & \langle 1|X|2\rangle & \cdots \\ \langle 2|X|1\rangle & \langle 2|X|2\rangle & \cdots \\ & \cdots & \end{pmatrix} \end{array}$$

: matrix representation of X in $|i\rangle$-basis.

$\rightarrow$ $Z = XY$: matrix multiplication.

$$\langle i|Z|j\rangle = \langle i|XY|j\rangle = \sum_k \langle i|X|k\rangle\langle k|Y|j\rangle$$

$\rightarrow$ $|\gamma\rangle = X|\alpha\rangle$: matrix-vector multiplication

$$\langle i|\gamma\rangle = \langle i|X|\alpha\rangle$$

$$= \sum_j \langle i|X|j\rangle\langle j|\alpha\rangle$$

$X \qquad \doteq |\alpha\rangle$

$|\gamma\rangle$ $\doteq$ col. vec

$$\Rightarrow \begin{pmatrix} \langle 1|\gamma\rangle \\ \langle 2|\gamma\rangle \\ \vdots \end{pmatrix} = \begin{pmatrix} \diagdown & & \\ & X_{ij} & \\ & & \diagdown \end{pmatrix} \begin{pmatrix} \langle 1|\alpha\rangle \\ \langle 2|\alpha\rangle \\ \vdots \end{pmatrix}$$

Likewise, bra $\langle\gamma| = \langle\alpha| X$

$\Rightarrow$ $\underbrace{\langle\gamma|j\rangle}_{\doteq\langle\gamma|} = \sum_i \underbrace{\langle\alpha|i\rangle}_{\doteq\langle\alpha|}\underbrace{\langle i|X|j\rangle}_{\doteq X}$

$\Rightarrow$ $(\underbrace{\langle\gamma|1\rangle}_{=\langle 1|\gamma\rangle^*}, \underbrace{\langle\gamma|2\rangle}_{=\langle 2|\gamma\rangle^*}, \cdots) = (\underbrace{\langle\alpha|1\rangle}_{=\langle 1|\alpha\rangle^*}, \underbrace{\langle\alpha|2\rangle}_{=\langle 2|\alpha\rangle^*}, \cdots)\begin{pmatrix} \ddots & & \\ & X_{ij} & \\ & & \ddots \end{pmatrix}$

" row-vector = row-vec. x Matrix "

$\Rightarrow$ inner product. $\langle\beta|\alpha\rangle = \sum_i \langle\beta|i\rangle\langle i|\alpha\rangle$

$$= (\langle 1|\beta\rangle^*, \langle 2|\beta\rangle^*, \cdots)\begin{pmatrix} \langle 1|\alpha\rangle \\ \langle 2|\alpha\rangle \\ \vdots \end{pmatrix}$$

as we expect.

$\Rightarrow$ outer product. $|\beta\rangle\langle\alpha|$: just an operator!

$$|\beta\rangle\langle\alpha| = I \cdot |\beta\rangle\langle\alpha| \cdot I$$

$$= \sum_{ij} |i\rangle \underbrace{\langle i|\beta\rangle\langle\alpha|j\rangle}\langle j|$$

Matrix

$$= \begin{array}{c|c} & j \rightarrow \\ \hline i \downarrow & \begin{pmatrix} \langle 1|\beta\rangle\langle 1|\alpha\rangle^* & \langle 1|\beta\rangle\langle 2|\alpha\rangle^* & \cdots \\ \langle 2|\beta\rangle\langle 1|\alpha\rangle^* & \langle 2|\beta\rangle\langle 2|\alpha\rangle^* & \cdots \\ & & \ddots \end{pmatrix} \end{array}$$

special case

$\Rightarrow$ Eigenkets of A as the base ket.

$$A = \sum_{ij} |i\rangle\underbrace{\langle i|A|j\rangle}\langle j|$$

$\hookrightarrow$ $\langle i|A|j\rangle = a_i\,\delta_{ij}$.

$\Rightarrow$ $A = \sum_i a_i |i\rangle\langle i| = \sum_i a_i \Lambda_i$

* How to choose the base kets?

- No general Rule... It's usually done by inspection.

- Eigenkets of a physical observable in the H-space that you consider.

"Known"

ex. In continuum, (position / momentum) operators

"obvious" eigenkets
$|x\rangle$, $|p\rangle$ $\xrightarrow{\text{def.}}$ wave functions

$\psi(x) = \langle x|\psi\rangle$, $\phi(p) = \langle p|\psi\rangle$

orthogonality

$\langle x'|x\rangle = \delta_{x'x}$, likewise for p.

ex. ~~In~~ Spin-$\frac{1}{2}$ systems.

: $|\uparrow\rangle, |\downarrow\rangle$

← Eigenkets of S_z.

ex: Atomic lattice (a single-particle regime)

→ atomic basis $|n\rangle$. (single orbital)

→ orbital basis (s, p, d, ... : "non-orthogonal")

(4) Example : a spin-$\frac{1}{2}$ system.

Eigenstates of S_z-operator : $\begin{pmatrix} |S_z;+\rangle \equiv |\uparrow\rangle \\ |S_z;-\rangle \equiv |\downarrow\rangle \end{pmatrix}$.

Let $|\uparrow\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\quad |\downarrow\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

✓ Completeness : $\mathbb{1} = |\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|$

$$= \begin{pmatrix} 1 \\ 0 \end{pmatrix}(1\ 0) + \begin{pmatrix} 0 \\ 1 \end{pmatrix}(0\ 1)$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

eigenvalues of S_z operator in the spin-$\frac{1}{2}$ system.

$$S_z|\uparrow\rangle = \frac{\hbar}{2}|\uparrow\rangle, \quad S_z|\downarrow\rangle = -\frac{\hbar}{2}|\downarrow\rangle \qquad \text{(SG exp.)}$$

$$\Rightarrow \quad S_z \doteq \begin{pmatrix} \frac{\hbar}{2} & 0 \\ 0 & -\frac{\hbar}{2} \end{pmatrix}.$$

- other operators : useful.

$$S_+ \equiv \hbar|\uparrow\rangle\langle\downarrow|, \quad S_- = \hbar|-\rangle\langle+|$$

$$\doteq \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad \doteq \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

1.4 Measurements, observables, and the uncertainty relations

(1) Measurements (on a "pure" state)

Dirac 1958 : " A measurement always causes the system to jump into an eigenstate of the dynamical variable that is being measured ".

$\Rightarrow$ measurement is projective.

ex. measuring an observable associated to an op. "A".

$$A = \sum_i a_i |i\rangle\langle i|, \quad I = \sum_i |i\rangle\langle i|$$

- Before the measurement, the system is at $|\alpha\rangle$.

$$|\alpha\rangle = \sum_a C_i|i\rangle = \sum_i |i\rangle\langle i|\alpha\rangle$$

- Do the measurement : $|\alpha\rangle \xrightarrow{\text{with some probability}} |i\rangle$. !

~~tex.~~ (exception) (when the system is at an eigenstate !) & $|i\rangle \rightarrow |i\rangle$ (unchanged)

- probability for jumping into a particular $|i\rangle$

$$= |\langle i|\alpha\rangle|^2 \qquad \| \qquad \sum_i |\langle i|\alpha\rangle|^2 = 1$$

- expectation value of A (w.r.t. $|\alpha\rangle$).

$$\langle A\rangle = \langle\alpha|A|\alpha\rangle$$

($\doteq$ averaged measured value.)

$$\Rightarrow \quad \langle A\rangle = \sum_{ij} \langle\alpha|i\rangle \underbrace{\langle i|A|j\rangle}_{a_i \delta_{ij}} \langle j|\alpha\rangle$$

$$= \sum_i a_i \; |\langle i|\alpha\rangle|^2$$

$|\langle i|\alpha\rangle|^2$ ← prob.

a_i ← measured value

← This is for a "pure" state. ← What we're considering mostly in this course.

: for repeated measurements, all systems are prepared at the same $|\alpha\rangle$.

c.f. "mixed" states (ex. thermal)

- generalization : a density operator. ρ ← We're coming back to this later

pure state : $\rho = |\Psi\rangle\langle\Psi|$

otherwise, it's a mixed state

↳ expectation value $\langle A\rangle = \mathrm{Tr}[\rho A]$

ex. pure state $\rho = |\alpha\rangle\langle\alpha|$

$$\Rightarrow \mathrm{Tr}[\,|\alpha\rangle\langle\alpha| A\,] = \langle\alpha|A|\alpha\rangle$$

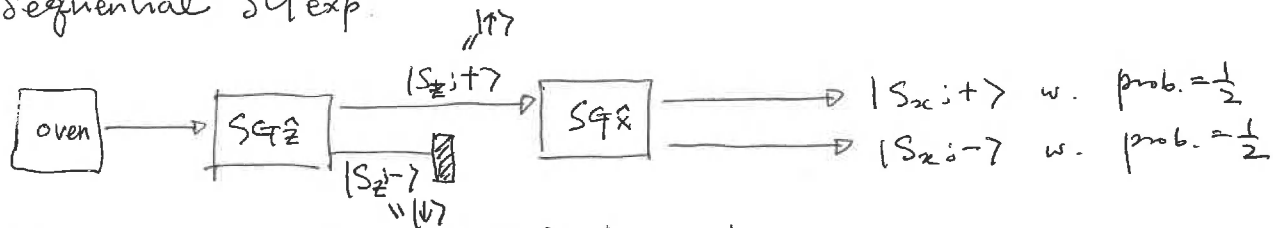
(2) spin-$\frac{1}{2}$ system : a review.

- Write everything in $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis.

$\Rightarrow$ $|S_x;\pm\rangle$, $|S_y;\pm\rangle$, S_x, S_y, $\vec{S}^2 = S_x^2 + S_y^2 + S_z^2$

- $|S_x;\pm\rangle$

Sequential SG exp.



It's the same for $|S_z;-\rangle$ being chosen.

$$\Rightarrow \quad |\langle\uparrow|S_x;\pm\rangle| = |\langle\downarrow|S_x;\pm\rangle| = \frac{1}{\sqrt{2}}$$

Therefore, some phase factor.

$$|S_x;+\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle + \frac{1}{\sqrt{2}}e^{i\delta_1}|\downarrow\rangle$$

$$|S_x;-\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle - \frac{1}{\sqrt{2}}e^{i\delta_1}|\downarrow\rangle$$

$\hookrightarrow$ $\langle S_x;+|S_x;-\rangle = 0$
orthogonality condition.

- S_x operator.
  : eigenvalues $\frac{\hbar}{2}$, $-\frac{\hbar}{2}$ in $|S_x;+\rangle$, $|S_x;-\rangle$ basis

$$S_x = \frac{\hbar}{2}\Big[\big(|S_x;+\rangle\langle S_x;+|\big) - \big(|S_x;-\rangle\langle S_x;-|\big)\Big]$$

$$= \frac{\hbar}{2}\left[e^{-i\delta_1}|\uparrow\rangle\langle\downarrow| + e^{i\delta_1}|\downarrow\rangle\langle\uparrow|\right]$$

- likewise for S_y

$$|S_y;\pm\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle \pm \frac{1}{\sqrt{2}}e^{i\delta_2}|\downarrow\rangle$$

$$S_y = \frac{\hbar}{2}\left[e^{-i\delta_2}|\uparrow\rangle\langle\downarrow| + e^{i\delta_2}|\downarrow\rangle\langle\uparrow|\right]$$

- How to determine δ_1, δ_2 ?

Rotate the SG axis.

$$\Rightarrow \quad |\langle S_y;\pm|S_x;+\rangle| = |\langle S_y;\pm|S_x;-\rangle| = \frac{1}{\sqrt{2}}$$

$$\Rightarrow \quad \frac{1}{2}\left|1 \pm e^{i(\delta_1-\delta_2)}\right| = \frac{1}{\sqrt{2}}.$$

$$\therefore \quad \delta_1 - \delta_2 = \frac{\pi}{2} \text{ or } -\frac{\pi}{2}$$

Let's just choose δ_1 to make all matrix element of S_z to be **REAL**.

$$\Rightarrow \quad \delta_1 = 0, \quad \delta_2 = \frac{\pi}{2}$$

$\pm\frac{\pi}{2}$ is possible, but $\frac{\pi}{2}$ is correct for Right-handed system.

(wait for ch. 3).

$$|S_x;\pm\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle \pm \frac{1}{\sqrt{2}}|\downarrow\rangle$$

$$|S_y;\pm\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle \pm \frac{i}{\sqrt{2}}|\downarrow\rangle$$

$$S_x = \frac{\hbar}{2}\left[\,|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\,\right] \rightarrow \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$S_y = \frac{\hbar}{2}\left[-i\,|\uparrow\rangle\langle\downarrow| + i\,|\downarrow\rangle\langle\uparrow|\right] \rightarrow \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

- $S_\pm$ operators ; $S_\pm = S_x \pm i S_y$. (raising / lowering operators)

- Commutation, anti-commutation relation.

$$[S_i, S_j] = i\,\varepsilon_{ijk}\hbar S_k, \quad \{S_i, S_j\} = \frac{1}{2}\hbar^2\delta_{ij}$$

* $[A,B] = AB - BA$, $\{A,B\} = AB + BA$

$$\varepsilon_{ijk} = \begin{cases} +1 & (ijk = (123) \text{ and any permutation}) \\ -1 & (ijk = (213) \text{ and any permutation}) \\ 0 & (\text{overlap of indices}) \end{cases}$$

levi-civita.

- $\vec{S}^2 = S_x^2 + S_y^2 + S_z^2 = \underline{\underline{\left(\frac{3}{4}\right)\hbar^2 \cdot \mathbb{1}}}$ ← just compute!

$\Rightarrow \left[\vec{S}^2, S_i\right] = 0$. ↑ only for spin-$\frac{1}{2}$.

↑ holds for any spin-S.

(3) Compatible Observables

def.
- compatible : commuting! $[A, B] = 0$. (ex. $[\vec{S}^2, S_z]$)
- incompatible : non-commuting! $[A, B] \neq 0$. (ex. $[S_x, S_y]$)

Let's start with <u>Theorem</u> :

If $[A, B] = 0$, the eigenvalues of A are $\underline{\underline{\text{non}}}$degenerate ,

‖ eigenkets $|a\rangle \Leftrightarrow a$ (eigenval.)

$\Rightarrow \langle a''|B|a'\rangle =$ "diagonal"

$\propto \delta_{a'a''}$.

<u>proof</u>.

$$\langle a''|[A, B]|a'\rangle = (a'' - a')\langle a''|B|a'\rangle = 0 .$$

$$\Rightarrow \langle a''|B|a'\rangle = 0 \quad \text{unless } a' = a'' .$$

☆ Eigenkets diagonalizing A

diagonalizes B as well if $[A, B] = 0$.

"This is also valid even if it (A or B) has <u>degeneracy</u> (eigenvals)."

☆☆☆

$$\boxed{\Rightarrow [A, B] \Rightarrow \text{There is a set of "Simultaneous" eigenkets of } A, B}$$

· Notation $A|a',b'\rangle = a'|a',b'\rangle$

$B|a',b'\rangle = b'|a',b'\rangle$

b' is not relevant

a' is not relevant.

← This is an overkill if there is no degeneracy.

But, it's extremely useful when there is degeneracy.

ex. $[L^2, L_z] = 0$

↳ $\hbar^2 l(l+1)$ → for l, $m = -l, \cdots l$.

↳ $|K\rangle \equiv |l, m\rangle$. ~~specifies~~ characterizes all orbital angular-momentum states.

Thus, it is very important to ~~know~~ find (well, if one can find) ...

" a maximal set " of commuting observable.

$[A,B] = [B,C] = [A,C] = \cdots = 0$.

$\Rightarrow |K'\rangle = |a', b', c', \cdots\rangle$

best characterizes the system!

↳ of course, it satisfies orthonormality

completeness.

$\langle K''|K'\rangle = \delta_{a''a'}\delta_{b''b'}\cdots$

$\sum_{K'} |K'\rangle\langle K'| = \sum_{a',b',c',\cdots} |a',b',c',\cdots\rangle\langle a',b',c',\cdots| = 1$.